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# 半線形波動方程式に対するスタッガード Runge-Kutta スキーム Staggered Runge-Kutta schemes for Semilinear Wave Equations

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## Abstract

A staggered Runge-Kutta (staggered RK) scheme is the time integration Runge-Kutta type scheme based on staggered grid, which was proposed by Ghrist and Fornberg and Driscoll in 2000. Afterwards, Vewer presented efficiency of the scheme for linear and semilinear wave equations through numerical experiments. We study stability and convergence properties of this scheme for semilinear wave equations. In particular, we prove convergence of a fully discrete scheme obtained by applying the staggered RK scheme to the MOL approximation of the equation.

Keywords: wave equation, staggered Runge-Kutta schemes, convergence

## 1 Introduction

We consider initial-boundary value problems of the form

$$\begin{aligned}\frac{\partial^2 u}{\partial t^2} &= D\Delta u + g(t, x, u), \quad 0 \leq t \leq T, \quad x \in \Omega, \\ u(t, x) &= \varphi(t, x), \quad 0 \leq t \leq T, \quad x \in \partial\Omega, \\ u(0, x) &= u_0(x), \quad \frac{\partial u}{\partial t}(0, x) = v_0(x), \quad x \in \Omega.\end{aligned}$$

Here  $u(t, x)$  is an  $\mathbb{R}$ -valued unknown function,  $\Omega$  is a bounded domain in  $\mathbb{R}^i, i = 1, 2, 3$  with the boundary  $\partial\Omega$ ,  $\Delta$  is the Laplace operator,  $D$  is a positive constant, and  $g(x, t, u)$  is an  $\mathbb{R}$ -valued given function. Also,  $u_0(x)$ ,  $v_0(x)$ ,  $\varphi(t, x)$  are given functions.

Many important wave equations, such as the Klein-Gordon equation (see, e.g., [10], [19]) and the nonlinear Klein-Gordon equation (see [17]), are represented in this form.

To apply numerical schemes, we may use the form

$$\begin{aligned}\frac{\partial u}{\partial t} &= v, \quad \frac{\partial v}{\partial t} = D\Delta u + g(t, x, u), \quad 0 \leq t \leq T, \quad x \in \Omega, \\ u(t, x) &= \varphi(t, x), \quad 0 \leq t \leq T, \quad x \in \partial\Omega, \\ u(0, x) &= u_0(x), \quad v(0, x) = v_0(x), \quad x \in \Omega.\end{aligned}\tag{1}$$

A well-known approach in the numerical solution of wave problems in partial differential equations (PDEs) is the method of lines (MOL) (see [12]). In this approach, PDEs are first discretized in space by finite difference or finite element techniques to be converted into a system of ordinary differential equations (ODEs).

Let  $\Omega_h$  be a grid with mesh width  $h > 0$ , and  $\mathbf{V}_h$  be the vector space of all functions from  $\Omega_h$  to  $\mathbb{R}$ . An MOL approximation of (1) is written in the form

$$\frac{du_h(t)}{dt} = v_h(t), \quad \frac{dv_h(t)}{dt} = DL_h u_h(t) + \varphi_h(t) + g_h(t, u_h(t)). \quad (2)$$

Here  $u_h, v_h$  are approximation functions of  $u$  and  $v$  such that  $u_h(t), v_h(t) \in \mathbf{V}_h$  for  $t \in [0, T]$ ,  $L_h$  is a difference approximation of  $\Delta$ ,  $g_h$  is a function from  $[0, T] \times \mathbf{V}_h$  to  $\mathbf{V}_h$  defined by  $g_h(t, u_h)(x) = g(t, x, u_h(t))$ ,  $x \in \Omega_h$ , for  $t \in [0, T]$ ,  $u_h \in \mathbf{V}_h$ , and  $\varphi_h(t)$  is a function determined from the boundary condition.

For the time integration of (2), Ghrist et al. [5] have proposed a staggered Runge-Kutta (staggered RK) scheme for semi-discrete wave equations which uses staggering in time. Spatial grid staggering is well-known. For example, the FDTD scheme (see [18]) in the electromagnetic field analysis and the SMAC scheme (see, e.g., [3, 9]) in the fluid calculation use space staggering. Ghrist et al, [5] have proposed and analyzed a fourth-order time-staggered scheme (RKS4) which can be viewed as an extension of an existing second-order time-staggered scheme along the idea of RK methods. This scheme has further been examined by Verwer [15, 16].

As is well known, RK approximations for PDEs suffer from order reduction phenomena. That is, the order of time-stepping in the fully discrete scheme is, in general, less than that of the underlying RK scheme (see, e.g., [8], [11], [14] on order reduction phenomena of RK schemes in the PDE context). Verwer [15] has observed that in the PDE context the order of RKS4 is equal to three. He also gives an analysis of this phenomenon.

In this paper, we study stability and convergence of staggered RK schemes for (2). Specifically, we introduce a new stability condition which guarantees the boundedness of numerical solutions and prove convergence of the schemes.

The paper is organized as follows. In the next section (Section 2), we introduce some notation, including the form of the staggered RK schemes. In Section 3, we prove a theorem on the boundedness of the numerical solution. In Section 4, we prove a theorem on convergence of the scheme applied to (2). In Section 5, we numerically estimate the order of convergence through a numerical experiment.

## 2 Preliminaries

Let  $\tau > 0$  be a step size. We define the step points  $t_n = n\tau$ ,  $t_{n+1/2} = (n + 1/2)\tau$  for integer  $n \geq 0$ .

As described in [5], for positive integer  $s$ , a staggered RK scheme for ODEs of the form

$$\begin{cases} u' = f(t, v) \\ v' = g(t, u) \end{cases}, \quad 0 \leq t \leq T, \quad u, v \in \mathbb{R} \quad (3)$$

is given by

$$\begin{aligned} v_{n+1/2,1} &= v_{n+1/2}, \\ u_{n,i} &= u_n + \tau \sum_{j=1}^i b_{i,j} f(t_{n+1/2} + e_j \tau, v_{n+1/2,j}), \quad i = 1, \dots, s-1, \\ v_{n+1/2,i} &= v_{n+1/2} + \tau \sum_{j=1}^{i-1} a_{i,j} g(t_n + c_j \tau, u_{n,j}), \quad i = 2, \dots, s, \end{aligned} \quad (4)$$

$$\begin{aligned} u_{n+1} &= u_n + \tau \sum_{i=1}^s d_i f(t_{n+1/2} + e_i \tau, v_{n+1/2,i}), \\ u'_{n+1,1} &= u_{n+1}, \\ v'_{n+1/2,i} &= v_{n+1/2} + \tau \sum_{j=1}^i b'_{i,j} g(t_{n+1} + e'_j \tau, u'_{n+1,j}), \quad i = 1, \dots, s-1, \\ u'_{n+1,i} &= u_{n+1} + \tau \sum_{j=1}^{i-1} a'_{i,j} f(t_{n+1/2} + c'_j \tau, v'_{n+1/2,j}), \quad i = 2, \dots, s, \\ v_{n+3/2} &= v_{n+1/2} + \tau \sum_{i=1}^s d'_i g(t_{n+1} + e'_i \tau, u'_{n+1,i}) \end{aligned} \quad (5)$$

with the abscissae

$$\begin{aligned} c_i &= \sum_{j=1}^i b_{i,j}, \quad c'_i = \sum_{j=1}^i b'_{i,j}, \quad i = 1, \dots, s-1, \\ e_i &= \sum_{j=1}^{i-1} a_{i,j}, \quad e'_i = \sum_{j=1}^{i-1} a'_{i,j}, \quad i = 2, \dots, s. \end{aligned} \quad (6)$$

Here  $a_{i,j}$ ,  $b_{i,j}$ ,  $a'_{i,j}$ ,  $b'_{i,j}$ ,  $c_i$ ,  $c'_i$ ,  $d_i$ ,  $d'_i$ ,  $e_i$ ,  $e'_i$  are coefficients,  $e_1 = e'_1 = 0$ ,  $u_{n,i}$ ,  $v_{n+1/2,i}$ ,  $u'_{n+1,i}$ ,  $v'_{n+1/2,i}$  are intermediate variables,  $u_n$  and  $v_{n+1/2}$  are approximate values of  $u(t_n)$  and  $v(t_{n+1/2})$ , respectively.

We describe the algorithm of the staggered RK scheme. In the first step, we calculate  $u_1$  from  $u_0$  and  $v_{1/2}$  by (4), where  $v_{1/2}$  is produced from given initial values  $u_0(x) = u_0$ ,  $v_0(x) = v_0$ ,  $x \in \Omega_h$  and using a traditional explicit Runge-Kutta scheme. During

the next step, we calculate  $v_{3/2}$  from  $v_{1/2}$  and  $u_1$  by (5). So, generally, we calculate  $u_{n+1}$  from  $u_n$  and  $v_{n+1/2}$  by (4), and  $v_{n+3/2}$  from  $v_{n+1/2}$  and  $u_{n+1}$  by (5) and all approximate values are calculated explicitly.

We introduce some notation. The  $m \times m$  identity matrix will be denoted by  $I_m$ . We use the standard symbol  $\mathbf{1} = (1, \dots, 1)^T \in \mathbb{R}^s$ . To analyze stability of the scheme, we use the following linear test equation:

$$\begin{cases} u'(t) = v(t) \\ v'(t) = -\omega^2 u(t) \end{cases}, \quad \omega > 0 \quad (7)$$

where  $u(t)$  is an  $\mathbb{R}$ -valued function.

Applying (4)-(5) to (7), we get

$$\begin{aligned} V_{n+1/2} &= \mathbf{1}v_{n+1/2} - \tau\omega^2 AU_n, \\ U_n &= \mathbf{1}u_n + \tau BV_{n+1/2}, \\ u_{n+1} &= u_n + \tau dV_{n+1/2}, \\ U'_{n+1} &= \mathbf{1}u_{n+1} + \tau A'V'_{n+1/2}, \\ V'_{n+1/2} &= \mathbf{1}v_{n+1/2} - \tau\omega^2 B'U'_{n+1}, \\ v_{n+3/2} &= v_{n+1/2} - \tau\omega^2 d'U'_{n+1}, \end{aligned} \quad (8)$$

where

$$\begin{aligned} A &= \begin{pmatrix} 0 & & & \\ a_{2,1} & 0 & & O \\ \vdots & \ddots & \ddots & \\ a_{s,1} & \cdots & a_{s,s-1} & 0 \end{pmatrix}, \quad B = \begin{pmatrix} b_{1,1} & & & \\ b_{2,1} & b_{2,2} & & O \\ \vdots & \vdots & \ddots & \\ b_{s,1} & b_{s,2} & \cdots & b_{s,s} \end{pmatrix}, \quad d = \begin{pmatrix} d_1 \\ d_2 \\ \vdots \\ d_s \end{pmatrix}^T, \\ A' &= \begin{pmatrix} 0 & & & \\ a'_{2,1} & 0 & & O \\ \vdots & \ddots & \ddots & \\ a'_{s,1} & \cdots & a'_{s,s-1} & 0 \end{pmatrix}, \quad B' = \begin{pmatrix} b'_{1,1} & & & \\ b'_{2,1} & b'_{2,2} & & O \\ \vdots & \vdots & \ddots & \\ b'_{s,1} & b'_{s,2} & \cdots & b'_{s,s} \end{pmatrix}, \quad d' = \begin{pmatrix} d'_1 \\ d'_2 \\ \vdots \\ d'_s \end{pmatrix}^T, \\ V_{n+1/2} &= (v_{n+1/2,1}, v_{n+1/2,2}, \dots, v_{n+1/2,s})^T, \quad U_n = (u_{n,1}, u_{n,2}, \dots, u_{n,s})^T, \\ V'_{n+1/2} &= (v'_{n+1/2,1}, v'_{n+1/2,2}, \dots, v'_{n+1/2,s})^T, \\ U'_{n+1} &= (u'_{n+1,1}, u'_{n+1,2}, \dots, u'_{n+1,s})^T. \end{aligned}$$

Eliminating  $V_{n+1/2}$ ,  $U_n$ ,  $U'_{n+1}$  and  $V'_{n+1/2}$ , we can rewrite (8) as

$$\begin{pmatrix} u_{n+1} \\ v_{n+3/2} \end{pmatrix} = \begin{pmatrix} \omega & 0 \\ 0 & 1 \end{pmatrix}^{-1} R(\tau\omega) \begin{pmatrix} \omega & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} u_n \\ v_{n+1/2} \end{pmatrix}. \quad (9)$$

For  $\theta \geq 0$ ,  $R(\theta)$  is given by

$$R(\theta) = \begin{pmatrix} 1 + r_{1,1}(\theta)\mathbf{1} & r_{1,2}(\theta)\mathbf{1} \\ r'_{1,2}(\theta)\mathbf{1}(r_{1,1}(\theta)\mathbf{1} + 1) & 1 + r'_{1,2}(\theta)\mathbf{1}r_{1,2}(\theta)\mathbf{1} + r'_{1,1}(\theta)\mathbf{1} \end{pmatrix} \quad (10)$$

with

$$\begin{aligned} r_{1,1}(\theta) &= -\theta^2 d(I_s + \theta^2 AB)^{-1} A, & r_{1,2}(\theta) &= \theta d(I_s + \theta^2 AB)^{-1}, \\ r'_{1,1}(\theta) &= -\theta^2 d'(I_s + \theta^2 A'B')^{-1} A', & r'_{1,2}(\theta) &= -\theta d'(I_s + \theta^2 A'B')^{-1}. \end{aligned}$$

Noticing  $(\theta^2 AB)^s = O$  and  $(\theta^2 A'B')^s = O$ , we get

$$(I_s + \theta^2 AB)^{-1} = \sum_{i=0}^{s-1} (-\theta^2 AB)^i, \quad (I_s + \theta^2 A'B')^{-1} = \sum_{i=0}^{s-1} (-\theta^2 A'B')^i$$

with  $(-\theta^2 AB)^0 = (-\theta^2 A'B')^0 = I_s$ . Then we rewrite the coefficients in (10) as

$$\begin{aligned} r_{1,1}(\theta) &= d \sum_{i=0}^{s-1} (-\theta^2)^{i+1} (AB)^i A, & r_{1,2}(\theta) &= d \sum_{i=0}^{s-1} (-\theta^2)^i \theta (AB)^i, \\ r'_{1,1}(\theta) &= d' \sum_{i=0}^{s-1} (-\theta^2)^{i+1} (A'B')^i A', & r'_{1,2}(\theta) &= -d' \sum_{i=0}^{s-1} (-\theta^2)^i \theta (A'B')^i. \end{aligned} \quad (11)$$

Let  $\lambda_{\pm} = \lambda_{\pm}(\theta)$  be the eigenvalues of (10), which are the roots of

$$\begin{aligned} \lambda^2 - (2 + r_{1,1}(\theta)\mathbf{1} + r'_{1,1}(\theta)\mathbf{1} + r_{1,2}(\theta)\mathbf{1}r'_{1,2}(\theta)\mathbf{1})\lambda \\ + (1 + r_{1,1}(\theta)\mathbf{1})(1 + r'_{1,1}(\theta)\mathbf{1}) = 0. \end{aligned} \quad (12)$$

Under this notation, we define the stability interval of the scheme.

**Definition 1.** *The stability interval  $S$  of a staggered RK scheme (4)-(5) is defined by a connected closed interval of  $\{\theta; |\lambda_{\pm}(\theta)| \leq 1, \theta \geq 0\}$ , which includes 0.*

The simplest example of staggered RK schemes is the (staggered) leapfrog scheme (see, e.g., [15])

$$\begin{aligned} u_{n+1} &= u_n + \tau f(t_{n+1/2}, v_{n+1/2}), \\ v_{n+3/2} &= v_{n+1/2} + \tau g(t_{n+1}, u_{n+1}). \end{aligned} \quad (13)$$

This scheme is of order 2 for ODEs. In this case, the scheme applied to (7) is reduced to (9) with

$$r_{1,1}(\theta)\mathbf{1} = r'_{1,1}(\theta)\mathbf{1} = 0, \quad r_{1,2}(\theta)\mathbf{1} = \theta, \quad r'_{1,2}(\theta)\mathbf{1} = -\theta. \quad (14)$$

Substituting (14) into (12), we get  $\lambda^2 - (2 - \theta^2)\lambda + 1 = 0$ . Since the discriminant of  $\lambda^2 - (2 - \theta^2)\lambda + 1 = 0$  is  $D(\theta) = (2 - \theta^2)^2 - 4$ , it is easy to see that  $|\lambda_{\pm}(\theta)| \leq 1$  iff  $D(\theta) \leq 0$ .  $S$  is estimated by using the smallest positive root of  $-2 = 2 - \theta^2$ , i.e.  $S = [0, 2]$ .

RKS4 from [5] is another example of a staggered RK scheme. It is obtained by taking

$$A = A' = \begin{pmatrix} 0 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad B = B' = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad d = d' = \left( \frac{11}{12}, \frac{1}{24}, \frac{1}{24} \right). \quad (15)$$

This scheme is of order 4 for ODEs. In this case, the scheme for (7) is reduced to (9) with

$$r_{1,1}(\theta)\mathbf{1} = r'_{1,1}(\theta)\mathbf{1} = 0, \quad r_{1,2}(\theta)\mathbf{1} = \theta - \frac{\theta^3}{24}, \quad r'_{1,2}(\theta)\mathbf{1} = -\theta + \frac{\theta^3}{24}. \quad (16)$$

Substituting (16) into (12), we get

$$\lambda^2 - \left\{ 2 - (\theta - \theta^3/24)^2 \right\} \lambda + 1 = 0.$$

In [15],  $S$  is found to be defined by the smallest positive root of  $-2 = 2 - (\theta - \theta^3/24)^2$ , i.e.  $S = [0, 2(2^{1/3} + 2^{2/3})]$ .

### 3 Stability of staggered RK schemes

We use (9) to estimate the stability of the staggered RK scheme. In order to prove convergence of the staggered RK scheme in the next section, we have to evaluate  $\|R(\theta)^n\|_2$  of (10), where  $\|\cdot\|_2$  is the Euclidean norm on  $\mathbb{R}^2$  and the corresponding operator norm for  $2 \times 2$  matrices. To accomplish this evaluation, we define another stability interval.

Let  $\gamma_0 > 0$  ( $\gamma_0 \in S$ ) be the smallest positive root of

$$D(\theta) = r_{1,2}(\theta)\mathbf{1}r'_{1,2}(\theta)\mathbf{1}\{r_{1,2}(\theta)\mathbf{1}r'_{1,2}(\theta)\mathbf{1} + 4\} = 0. \quad (17)$$

By using this  $\gamma_0$ , we define another stability interval  $S' = [0, \gamma_0]$ . By Definition 1,  $S'$  is a subset in  $S$ . We prove the boundedness of  $\|R(\theta)^n\|_2$  by using the following hypotheses for the staggered RK scheme (4)-(5):

- (H1) For  $\theta \in S'$ ,  $0 \leq -r'_{1,2}(\theta)\mathbf{1} \leq r_{1,2}(\theta)\mathbf{1} \leq -\gamma_0 r'_{1,2}(\theta)\mathbf{1}$ .
- (H2) For  $\theta \in S'$ ,  $D(\theta) \leq 0$ .
- (H3) The polynomials  $r_{1,1}(\theta)\mathbf{1}$  and  $r'_{1,1}(\theta)\mathbf{1}$  are zero.

(H4) The following order condition holds:  $d\mathbf{1} = d'\mathbf{1} = 1$ .

The leapfrog scheme (13) and RKS4 (15) satisfy these hypotheses. Substituting (14) into (17), we can take  $\gamma_0 = 2$  and  $S' = [0, 2)$  for the leapfrog scheme. By (14), the leapfrog scheme satisfies (H1)-(H3). (H4) is checked by using (13). Similarly, we can take  $\gamma_0 = 2\sqrt{6}$  and  $S' = [0, 2\sqrt{6})$  for RKS4, by substituting (16) into (17). By (16), RKS4 satisfies (H1)-(H3). By (15), (H4) holds.

**Theorem 3.1.** *Let  $\gamma_\varepsilon > 0$  be  $\gamma_\varepsilon < \gamma_0$ . Assume that the coefficients  $a_{i,j}, a'_{i,j}, b_{i,j}, b'_{i,j}, c_i, c'_i, d_i, d'_i, e_i, e'_i$  in (4)-(5) satisfy (H1)-(H4). Then, there is a positive constant  $C$  such that*

$$\|R(\theta)^n\|_2 \leq C \quad (18)$$

holds for any  $0 \leq \theta \leq \gamma_\varepsilon$  and  $n \in \mathbb{N}$ . Here  $R(\theta)$  is the matrix of (10).

**Proof.** By (H3), we can rewrite

$$R(\theta) = \begin{pmatrix} 1 & r_{1,2}(\theta)\mathbf{1} \\ r'_{1,2}(\theta)\mathbf{1} & 1 + r_{1,2}(\theta)\mathbf{1}r'_{1,2}(\theta)\mathbf{1} \end{pmatrix}. \quad (19)$$

If  $\theta = 0$ ,  $R(\theta)$  is the identity matrix. Then (18) holds for  $C = 1$ . Let  $\theta > 0$ . We can diagonalize (19) as

$$R(\theta) = Q(\theta) \begin{pmatrix} \lambda_+(\theta) & 0 \\ 0 & \lambda_-(\theta) \end{pmatrix} Q(\theta)^{-1}. \quad (20)$$

Here

$$\begin{aligned} \lambda_\pm(\theta) &= \lambda_\pm = \frac{2 + r_{1,2}(\theta)\mathbf{1}r'_{1,2}(\theta)\mathbf{1} \pm \sqrt{D(\theta)}}{2}, \\ Q(\theta) &= \frac{1}{r'_{1,2}(\theta)\mathbf{1}} \begin{pmatrix} -\lambda_- + 1 & -\lambda_+ + 1 \\ r'_{1,2}(\theta)\mathbf{1} & r'_{1,2}(\theta)\mathbf{1} \end{pmatrix}, \\ Q(\theta)^{-1} &= \frac{1}{\lambda_+ - \lambda_-} \begin{pmatrix} r'_{1,2}(\theta)\mathbf{1} & \lambda_+ - 1 \\ -r'_{1,2}(\theta)\mathbf{1} & -\lambda_- + 1 \end{pmatrix}. \end{aligned} \quad (21)$$

Since  $\theta \in S$ , we have  $|\lambda_\pm| \leq 1$ . By (H2), the adjoint matrices of  $Q(\theta)$  and  $Q(\theta)^{-1}$  are

$$\begin{aligned} Q(\theta)^* &= \frac{1}{r'_{1,2}(\theta)\mathbf{1}} \begin{pmatrix} -\lambda_+ + 1 & r'_{1,2}(\theta)\mathbf{1} \\ -\lambda_- + 1 & r'_{1,2}(\theta)\mathbf{1} \end{pmatrix}, \\ (Q(\theta)^{-1})^* &= \frac{1}{\lambda_- - \lambda_+} \begin{pmatrix} r'_{1,2}(\theta)\mathbf{1} & -r'_{1,2}(\theta)\mathbf{1} \\ \lambda_- - 1 & -\lambda_+ + 1 \end{pmatrix}. \end{aligned}$$



Putting  $a(\theta) = (\lambda_+ - 1)(\lambda_- - 1)$  and  $b(\theta) = r'_{1,2}(\theta)\mathbf{1}\{\lambda_+ + \lambda_- - 2\}$ , we have

$$Q(\theta)^*Q(\theta) = \frac{1}{(r'_{1,2}(\theta)\mathbf{1})^2} \begin{pmatrix} a(\theta) + (r'_{1,2}(\theta)\mathbf{1})^2 & (\lambda_+ - 1)^2 + (r'_{1,2}(\theta)\mathbf{1})^2 \\ (\lambda_- - 1)^2 + (r'_{1,2}(\theta)\mathbf{1})^2 & a(\theta) + (r'_{1,2}(\theta)\mathbf{1})^2 \end{pmatrix},$$

$$(Q(\theta)^{-1})^*(Q(\theta)^{-1}) = \frac{-1}{\{\lambda_- - \lambda_+\}^2} \begin{pmatrix} 2r'_{1,2}(\theta)^2 & b(\theta) \\ b(\theta) & 2a(\theta) \end{pmatrix}.$$

Then, the eigenvalues of  $Q(\theta)^*Q(\theta)$  and  $(Q(\theta)^{-1})^*(Q(\theta)^{-1})$  are

$$\frac{a(\theta) + (r'_{1,2}(\theta)\mathbf{1})^2 \pm \sqrt{\{(\lambda_+ - 1)^2 + (r'_{1,2}(\theta)\mathbf{1})^2\}\{(\lambda_- - 1)^2 + (r'_{1,2}(\theta)\mathbf{1})^2\}}}{(r'_{1,2}(\theta)\mathbf{1})^2},$$

$$\frac{a(\theta) + (r'_{1,2}(\theta)\mathbf{1})^2 \pm \sqrt{(a(\theta) - (r'_{1,2}(\theta)\mathbf{1})^2)^2 + b(\theta)^2}}{-\{\lambda_- - \lambda_+\}^2},$$

respectively. Putting

$$\begin{aligned} \alpha(\theta) &= -r_{1,2}(\theta)\mathbf{1}r'_{1,2}(\theta)\mathbf{1} + (r'_{1,2}(\theta)\mathbf{1})^2, \\ \beta(\theta) &= r'_{1,2}(\theta)\mathbf{1}(\lambda_+ - \lambda_-)i, \end{aligned} \tag{22}$$

these eigenvalues are rewritten as

$$\frac{\alpha(\theta) \pm \sqrt{\alpha(\theta)^2 - \beta(\theta)^2}}{(r_{2,1}(\theta)\mathbf{1})^2}, \quad \frac{(r_{2,1}(\theta)\mathbf{1})^2 \left\{ \alpha(\theta) \pm \sqrt{\alpha(\theta)^2 - \beta(\theta)^2} \right\}}{\beta(\theta)^2},$$

respectively. Then, by (20), we have

$$\|R(\theta)^n\|_2 \leq \|Q(\theta)\|_2 \|Q(\theta)^{-1}\|_2 = \left| \frac{\alpha(\theta) + \sqrt{\alpha(\theta)^2 - \beta(\theta)^2}}{\beta(\theta)} \right| \leq 2 \left| \frac{\alpha(\theta)}{\beta(\theta)} \right| + 1. \tag{23}$$

Substituting (21) into (22) and using (H1), we have

$$\begin{aligned} \left| \frac{\alpha(\theta)}{\beta(\theta)} \right| &= \frac{|r_{1,2}(\theta)\mathbf{1} - r'_{1,2}(\theta)\mathbf{1}|}{\sqrt{-r'_{1,2}(\theta)\mathbf{1}r_{1,2}(\theta)\mathbf{1}(r_{1,2}(\theta)\mathbf{1}r'_{1,2}(\theta)\mathbf{1} + 4)}} \\ &\leq \frac{(1 + \gamma_0)r'_{1,2}(\theta)\mathbf{1}}{r'_{1,2}(\theta)\mathbf{1}\sqrt{r_{1,2}(\theta)\mathbf{1}r'_{1,2}(\theta)\mathbf{1} + 4}} \end{aligned}$$

for any  $\theta \in [0, \gamma_\epsilon]$ . By (H1) and (H2), we get  $-4 \leq r_{1,2}(\theta)\mathbf{1}r'_{1,2}(\theta)\mathbf{1} \leq 0$ . As  $r_{1,2}(\theta)\mathbf{1}r'_{1,2}(\theta)\mathbf{1}$  is a polynomial of  $\theta$ , there exists a minimum value of  $r_{1,2}(\theta)\mathbf{1}r'_{1,2}(\theta)\mathbf{1} +$

4 in  $[0, \gamma_\varepsilon]$ . Let  $\gamma_1$  be the value of  $\theta$  that gives the minimum value of  $r_{1,2}(\theta)\mathbf{1}r'_{1,2}(\theta)\mathbf{1} + 4$ . We get

$$\left| \frac{\alpha(\theta)}{\beta(\theta)} \right| \leq \frac{1 + \gamma_0}{\sqrt{r_{1,2}(\gamma_1)\mathbf{1}r_{2,1}(\gamma_1)\mathbf{1} + 4}}.$$

Then, this, together with (23), gives (18) with  $C = \frac{2(1 + \gamma_0)}{\sqrt{r_{1,2}(\gamma_1)\mathbf{1}r_{2,1}(\gamma_1)\mathbf{1} + 4}} + 1$ .  $\square$

## 4 Convergence of fully discrete schemes

We assume the following hypotheses for  $L_h$ :

$L_h$  is a negative definite symmetric matrix.

There exist  $h_0 > 0$  and  $C_3 > 0$  such that any eigenvalue of  $L_h$  is less than  $-C_3$  for any  $h < h_0$ .

By these hypotheses, there exists a positive definite symmetric matrix  $W_h$  satisfying  $-DL_h = W_h^2$ ; any eigenvalue of  $W_h^{-1}$  is less than  $1/\sqrt{DC_3}$  for any  $h < h_0$ . Then  $W_h^{-1}$  is bounded.

Using  $W_h$ , we can rewrite (2) as

$$\frac{du_h(t)}{dt} = v_h(t), \quad \frac{dv_h(t)}{dt} = -W_h^2 u_h(t) + \varphi_h(t) + g_h(t, u_h(t)). \quad (24)$$

In this paper,  $\|\cdot\|_{W_h}$  denotes a discrete energy norm (see, e.g., [1], [2]), given by

$$\|(u_h, v_h)^T\|_{W_h}^2 = \|W_h u_h\|^2 + \|v_h\|^2 \quad \text{for any } u_h, v_h \in \mathbf{V}_h, \quad (25)$$

where  $\|\cdot\|$  denotes the discrete version of the  $L_2$ -norm in  $\mathbf{V}_h$ , given by

$$\|u_h\|^2 = h \sum_{x \in \Omega_h} \{(u_h)_x\}^2$$

and the corresponding operator norm for  $m \times m$  matrices with  $m = \dim \mathbf{V}_h$ .

We define the spatial truncation error  $\alpha_h(t)$  (see, e.g., [6], I.4) by

$$\alpha_h(t) = \mathbf{v}'_h(t) + W_h^2 \mathbf{u}_h(t) - \varphi_h(t) - g_h(t, \mathbf{u}_h(t)), \quad (26)$$

where  $\mathbf{u}_h(t)$ ,  $\mathbf{v}_h(t)$  are  $\mathbf{V}_h$ -valued functions obtained by restricting the variable  $x$  of the exact solutions  $u$ ,  $v$  onto  $\Omega_h$ .

By applying (4)-(5) to (24), we obtain the following scheme for the problem (1):

$$\begin{aligned}
V_{n+1/2} &= \mathbf{1}' v_{n+1/2} + \tau \mathbf{A} \{-W_h^2 U_n + \varphi_h(t_n) + g_n\}, \\
U_n &= \mathbf{1}' u_n + \tau \mathbf{B} V_{n+1/2}, \\
u_{n+1} &= u_n + \tau d V_{n+1/2}, \\
U'_{n+1} &= \mathbf{1}' u_{n+1} + \tau \mathbf{A}' V'_{n+1/2}, \\
V'_{n+1/2} &= \mathbf{1}' v_{n+1/2} + \tau \mathbf{B}' \{-W_h^2 U'_{n+1} + \varphi_h(t_{n+1}) + g_{n+1}\}, \\
v_{n+3/2} &= v_{n+1/2} + \tau d' \{-W_h^2 U'_{n+1} + \varphi_h(t_{n+1}) + g_{n+1}\}.
\end{aligned} \tag{27}$$

Here  $\mathbf{1}'$  denotes  $\mathbf{1} \otimes I_m$  for  $\mathbf{1} = (1, \dots, 1)^T \in \mathbb{R}^s$ ,

$$\begin{aligned}
\mathbf{A} &= A \otimes I_m, \quad \mathbf{B} = B \otimes I_m, \quad \mathbf{d} = d \otimes I_m, \quad \mathbf{A}' = A' \otimes I_m, \quad \mathbf{B}' = B' \otimes I_m, \\
V_{n+1/2} &= (v_{n+1/2,1}^T, v_{n+1/2,2}^T, \dots, v_{n+1/2,s}^T)^T, \quad U_n = (u_{n,1}^T, u_{n,2}^T, \dots, u_{n,s}^T)^T, \\
V'_{n+1/2} &= (v_{n+1/2,1}'^T, v_{n+1/2,2}'^T, \dots, v_{n+1/2,s}'^T)^T, \\
U'_{n+1} &= (u_{n+1,1}'^T, u_{n+1,2}'^T, \dots, u_{n+1,s}'^T)^T, \\
\varphi_h(t_n) &= (\varphi_h(t_{n,1})^T, \varphi_h(t_{n,2})^T, \dots, \varphi_h(t_{n,s})^T)^T, \quad \mathbf{d}' = d' \otimes I_m, \\
g_n &= (g_h(t_{n,1}, u_{n,1})^T, g_h(t_{n,2}, u_{n,2})^T, \dots, g_h(t_{n,s}, u_{n,s})^T)^T, \quad W_h = I_s \otimes W_h
\end{aligned}$$

with  $\otimes$  standing for the Kronecker product (see, e.g., [4]),  $u_{n,i}$ ,  $v_{n+1/2,i}$ ,  $u'_{n+1,i}$  and  $v'_{n+1/2,i}$  are intermediate variables,  $t_{n,j} := t_n + c_j \tau$ ,  $t_{n+1,j} := t_{n+1} + c'_j \tau$ ,  $u_n$  and  $v_{n+1/2}$  are approximate values of  $u_h(t_n)$  and  $v_h(t_{n+1/2})$ , respectively.

For some  $s$ -dimensional vector  $\mathbf{a} = (a_1, \dots, a_s)^T$ , we define  $\mathbf{a}^i = (a_1^i, \dots, a_s^i)^T$ . In addition to the (H1)-(H4), we assume the following hypothesis for the staggered RK scheme (4)-(5):

(H5) The following order conditions hold:

$$\begin{aligned}
(A\mathbf{1})^2 + A\mathbf{1} &= 2AB\mathbf{1}, \quad (B\mathbf{1})^2 - B\mathbf{1} = 2BA\mathbf{1}, \\
(A'\mathbf{1})^2 + A'\mathbf{1} &= 2A'B'\mathbf{1}, \quad (B'\mathbf{1})^2 - B'\mathbf{1} = 2B'A'\mathbf{1}, \\
dA\mathbf{1} &= d'A'\mathbf{1} = 0.
\end{aligned}$$

The leapfrog scheme and RKS4 satisfy (H5), which is checked by (13) and (15). We assume the following condition which gives the restriction for  $\tau$  and  $h$ .

(H6)  $\tau \rho(W_h) \in S'$ . Here  $\rho(W_h)$  is the spectral radius of  $W_h$ .

Moreover, we assume the following condition for the problem (1):

The exact solution  $u(t, x)$  is of class  $C^4$  with respect to  $t$ ,  $g(t, x, u)$  is of class  $C^3$  with respect to  $t$ ,  $u$  and (each component of) the derivative  $\partial g / \partial u$  is bounded for  $(t, x, u) \in [0, T] \times \Omega \times \mathbb{R}$ .

For simplicity, we consider a step size of the form  $\tau = T/N$  with positive integer  $N$ . Then, we have the following theorem.

**Theorem 4.1.** Assume that the coefficients  $a_{i,j}$ ,  $a'_{i,j}$ ,  $b_{i,j}$ ,  $b'_{i,j}$ ,  $c_i$ ,  $c'_i$ ,  $d_i$ ,  $d'_i$ ,  $e_i$ ,  $e'_i$  in (4)-(5) satisfy (H1)-(H5) and  $\tau$  satisfies (H6). Then, there is a positive constant  $C_1$  such that

$$\left\| (\mathbf{u}_n - \mathbf{u}_h(t_n), \mathbf{v}_{n+1/2} - \mathbf{v}_h(t_{n+1/2}))^T \right\|_{W_h} \leq C_1 \left( \tau^2 + \max_{0 \leq t \leq T} \|\alpha_h(t)\| \right) \quad (28)$$

holds.

**Proof.** Put

$$\begin{aligned} \mathbf{V}_h(t_{n+1/2}) &= (\mathbf{v}_h(t_{n+1/2,1})^T, \mathbf{v}_h(t_{n+1/2,2})^T, \dots, \mathbf{v}_h(t_{n+1/2,s})^T)^T, \\ \mathbf{U}_h(t_n) &= (\mathbf{u}_h(t_{n,1})^T, \mathbf{u}_h(t_{n,2})^T, \dots, \mathbf{u}_h(t_{n,s})^T)^T, \\ \mathbf{V}_h(t'_{n+1/2}) &= (\mathbf{v}_h(t'_{n+1/2,1})^T, \mathbf{v}_h(t'_{n+1/2,2})^T, \dots, \mathbf{v}_h(t'_{n+1/2,s})^T)^T, \\ \mathbf{g}_h(t_n) &= (g_h(t_{n,1}, \mathbf{u}_h)^T, g_h(t_{n,2}, \mathbf{u}_h)^T, \dots, g_h(t_{n,s}, \mathbf{u}_h)^T)^T, \end{aligned}$$

where  $t_{n+1/2,j} := t_{n+1/2} + e_j\tau$ ,  $t'_{n+1/2,j} := t_{n+1/2} + e'_j\tau$ ,  $j = 1, \dots, s$ . Replacing  $\mathbf{U}_n$ ,  $\mathbf{U}'_{n+1}$ ,  $\mathbf{V}_{n+1/2}$ ,  $\mathbf{V}'_{n+1/2}$ ,  $\mathbf{u}_n$  and  $\mathbf{v}_{n+1/2}$  in the scheme (27) with  $\mathbf{U}_h(t_n)$ ,  $\mathbf{U}_h(t_{n+1})$ ,  $\mathbf{V}_h(t_{n+1/2})$ ,  $\mathbf{V}_h(t'_{n+1/2})$ ,  $\mathbf{u}_h(t_n)$  and  $\mathbf{v}_h(t_{n+1/2})$ , we obtain the recurrence relation

$$\begin{aligned} \mathbf{V}_h(t_{n+1/2}) &= \mathbf{1}' \mathbf{v}_h(t_{n+1/2}) + \tau \mathbf{A} \{-\mathbf{W}_h^2 \mathbf{U}_h(t_n) + \boldsymbol{\varphi}_h(t_n) + \mathbf{g}_h(t_n)\} + \mathbf{r}_{n+1/2}, \\ \mathbf{U}_h(t_n) &= \mathbf{1}' \mathbf{u}_h(t_n) + \tau \mathbf{B} \mathbf{V}_h(t_{n+1/2}) + \mathbf{r}_n, \\ \mathbf{u}_h(t_{n+1}) &= \mathbf{u}_h(t_n) + \tau \mathbf{d} \mathbf{V}_h(t_{n+1/2}) + \rho_n, \\ \mathbf{U}_h(t_{n+1}) &= \mathbf{1}' \mathbf{u}_h(t_{n+1}) + \tau \mathbf{A}' \mathbf{V}_h(t'_{n+1/2}) + \mathbf{r}_{n+1}, \\ \mathbf{V}_h(t'_{n+1/2}) &= \mathbf{1}' \mathbf{v}_h(t_{n+1/2}) + \tau \mathbf{B}' \{-\mathbf{W}_h^2 \mathbf{U}_h(t_{n+1}) + \boldsymbol{\varphi}_h(t_{n+1}) + \mathbf{g}_h(t_{n+1})\} + \mathbf{r}'_{n+1/2}, \\ \mathbf{v}_h(t_{n+3/2}) &= \mathbf{v}_h(t_{n+1/2}) + \tau \mathbf{d}' \{-\mathbf{W}_h^2 \mathbf{U}_h(t_{n+1}) + \boldsymbol{\varphi}_h(t_{n+1}) + \mathbf{g}_h(t_{n+1})\} + \rho_{n+1/2} \end{aligned} \quad (29)$$

with the residuals

$$\mathbf{r}_n = (r_{n,1}^T, r_{n,2}^T, \dots, r_{n,s}^T)^T, \quad \mathbf{r}'_{n+1/2} = (r'_{n+1/2,1}^T, r'_{n+1/2,2}^T, \dots, r'_{n+1/2,s}^T)^T,$$

$\rho_n$  and  $\rho_{n+1/2}$ . By (6), (26), (H4) and (H5), these residuals are expanded as

$$\begin{aligned} \mathbf{r}_{n+1/2} &= \tau^3 \boldsymbol{\zeta} \mathbf{v}_h^{(3)}(t_{n+1/2}) + \tau \mathbf{A} \boldsymbol{\alpha}_h(t_n) + O(\tau^4), \\ \mathbf{r}_n &= \tau^3 \boldsymbol{\eta} \mathbf{u}_h^{(3)}(t_n) + O(\tau^4), \\ \rho_n &= \frac{\tau^3}{2} \left( \frac{1}{12} - d(A\mathbf{1})^2 \right) \mathbf{u}_h^{(3)}(t_n) + O(\tau^4), \\ \mathbf{r}_{n+1} &= \tau^3 \boldsymbol{\zeta}' \mathbf{u}_h^{(3)}(t_{n+1}) + O(\tau^4), \\ \mathbf{r}'_{n+1/2} &= \tau^3 \boldsymbol{\eta}' \mathbf{v}_h^{(3)}(t_{n+1/2}) + \tau \mathbf{B}' \boldsymbol{\alpha}_h(t_{n+1}) + O(\tau^4), \\ \rho_{n+1/2} &= \frac{\tau^3}{2} \left( \frac{1}{12} - d'(A'\mathbf{1})^2 \right) \mathbf{v}_h^{(3)}(t_{n+1/2}) + \tau \mathbf{d}' \boldsymbol{\alpha}_h(t_{n+1}) + O(\tau^4). \end{aligned} \quad (30)$$

Here

$$\begin{aligned}
\alpha_h(t_n) &= (\alpha_h(t_{n,1})^T, \alpha_h(t_{n,2})^T, \dots, \alpha_h(t_{n,s})^T)^T, \\
\zeta &= \zeta \otimes I_m, \quad \eta = \eta \otimes I_m, \quad \zeta' = \zeta' \otimes I_m, \quad \eta' = \eta' \otimes I_m, \\
\zeta &= \frac{4(A\mathbf{1})^3 + 6(A\mathbf{1})^2 + 3(A\mathbf{1})}{24} - \frac{A(B\mathbf{1})^2}{2}, \\
\eta &= \frac{4(B\mathbf{1})^3 + 6(B\mathbf{1})^2 + 3(B\mathbf{1})}{24} - \frac{B(A\mathbf{1})^2}{2}, \\
\zeta' &= \frac{4(A'\mathbf{1})^3 + 6(A'\mathbf{1})^2 + 3(A'\mathbf{1})}{24} - \frac{A'(B'\mathbf{1})^2}{2}, \\
\eta' &= \frac{4(B'\mathbf{1})^3 + 6(B'\mathbf{1})^2 + 3(B'\mathbf{1})}{24} - \frac{B'(A'\mathbf{1})^2}{2}
\end{aligned}$$

and  $O(\tau^4)$  denotes a term whose component for each  $x \in \Omega_h$  is of  $O(\tau^4)$ . Subtracting (27) from (29), we obtain

$$\begin{aligned}
\delta_{n+1/2} &= \mathbf{1}'\varepsilon_{n+1/2} - \tau \mathbf{A}(\mathbf{W}_h^2 \delta_n - \mathbf{g}_h(t_n) + \mathbf{g}_n) + \mathbf{r}_{n+1/2}, \\
\delta_n &= \mathbf{1}'\varepsilon_n + \tau \mathbf{B}\delta_{n+1/2} + \mathbf{r}_n, \\
\varepsilon_{n+1} &= \varepsilon_n + \tau d\delta_{n+1/2} + \rho_n, \\
\delta'_{n+1} &= \mathbf{1}'\varepsilon_{n+1} + \tau \mathbf{A}'\delta'_{n+1/2} + \mathbf{r}_{n+1}, \\
\delta'_{n+1/2} &= \mathbf{1}'\varepsilon_{n+1/2} - \tau \mathbf{B}'(\mathbf{W}_h^2 \delta'_{n+1} - \mathbf{g}_h(t_{n+1}) + \mathbf{g}_{n+1}) + \mathbf{r}'_{n+1/2}, \\
\varepsilon_{n+3/2} &= \varepsilon_{n+1/2} - \tau d'(\mathbf{W}_h^2 \delta'_{n+1} - \mathbf{g}_h(t_{n+1}) + \mathbf{g}_{n+1}) + \rho_{n+1/2}.
\end{aligned}$$

Here

$$\begin{aligned}
\delta_{n+1/2} &= \mathbf{V}_h(t_{n+1/2}) - \mathbf{V}_{n+1/2}, \quad \delta_n = \mathbf{U}_h(t_n) - \mathbf{U}_n, \\
\delta'_{n+1} &= \mathbf{U}_h(t_{n+1}) - \mathbf{U}'_{n+1}, \quad \delta'_{n+1/2} = \mathbf{V}_h(t'_{n+1/2}) - \mathbf{V}'_{n+1/2}
\end{aligned}$$

and

$$\varepsilon_n = \mathbf{u}_h(t_n) - \mathbf{u}_n, \quad \varepsilon_{n+1/2} = \mathbf{v}_h(t_{n+1/2}) - \mathbf{v}_{n+1/2}.$$

Let  $\mathbf{J}_n$  be  $\mathbf{J}_n = \text{diag}(J_{n,1}, J_{n,2}, \dots, J_{n,s})$  and  $J_{n,i}$  be a function from  $\Omega_h$  to  $\mathbb{R}$  whose value for  $x \in \Omega_h$  is

$$J_{n,i}(x) = \int_0^1 \frac{\partial g}{\partial u}(t_{n,i}, x, (1-\theta)\mathbf{u}_{n,i}(x) + \theta\mathbf{u}_h(t_{n,i}, x)) d\theta.$$

By the assumption that  $\partial g / \partial u$  is bounded, there is a constant  $\gamma_3$  such that

$$\|J_{n,i}v\| \leq \gamma_3 \|v\| \quad \text{for any } v \in \mathbf{V}_h, \quad (31)$$

where the multiplication  $J_{n,i}v$  is component-wise for  $x \in \Omega_h$ . Then we obtain

$$\begin{aligned}\delta_{n+1/2} &= \mathbf{1}'\varepsilon_{n+1/2} - \tau\mathbf{A}(\mathbf{W}_h^2 - \mathbf{J}_n)\delta_n + \mathbf{r}_{n+1/2}, \\ \delta_n &= \mathbf{1}'\varepsilon_n + \tau\mathbf{B}\delta_{n+1/2} + \mathbf{r}_n, \\ \varepsilon_{n+1} &= \varepsilon_n + \tau\mathbf{d}\delta_{n+1/2} + \rho_n, \\ \delta'_{n+1} &= \mathbf{1}'\varepsilon_{n+1} + \tau\mathbf{A}'\delta'_{n+1/2} + \mathbf{r}_{n+1}, \\ \delta'_{n+1/2} &= \mathbf{1}'\varepsilon_{n+1/2} - \tau\mathbf{B}'(\mathbf{W}_h^2 - \mathbf{J}_{n+1})\delta'_{n+1} + \mathbf{r}'_{n+1/2}, \\ \varepsilon_{n+3/2} &= \varepsilon_{n+1/2} - \tau\mathbf{d}'(\mathbf{W}_h^2 - \mathbf{J}_{n+1})\delta'_{n+1} + \rho_{n+1/2}.\end{aligned}$$

Eliminating  $\delta_n$ ,  $\delta_{n+1/2}$ ,  $\delta'_{n+1/2}$  and  $\delta'_{n+1}$ , we have

$$\begin{pmatrix} W_h\varepsilon_{n+1} \\ \varepsilon_{n+3/2} \end{pmatrix} = \mathbf{R}_n \begin{pmatrix} W_h\varepsilon_n \\ \varepsilon_{n+1/2} \end{pmatrix} + \mathbf{M}_n \begin{pmatrix} W_h\xi_n \\ \xi_{n+1/2} \end{pmatrix}. \quad (32)$$

Here

$$\begin{aligned}\mathbf{R}_n &= \begin{pmatrix} I_m + R_{1,1}\mathbf{1}' & R_{1,2}\mathbf{1}' \\ R'_{1,2}\mathbf{1}'R_{1,1}\mathbf{1}' + R'_{1,2}\mathbf{1}' & I_m + R'_{1,2}\mathbf{1}'R_{1,2}\mathbf{1}' + R'_{1,1}\mathbf{1}' \end{pmatrix}, \quad \mathbf{M}_n = \begin{pmatrix} I_m & O \\ R'_{1,2}\mathbf{1}' & I_m \end{pmatrix}, \\ R_{1,1} &= -\tau^2\mathbf{d}(\mathbf{I} + \tau^2\mathbf{A}(\mathbf{W}_h^2 - \mathbf{J}_n)\mathbf{B})^{-1}\mathbf{A}(\mathbf{W}_h^2 - \mathbf{J}_n), \\ R_{1,2} &= \tau\mathbf{d}(\mathbf{I} + \tau^2\mathbf{A}(\mathbf{W}_h^2 - \mathbf{J}_n)\mathbf{B})^{-1}\mathbf{W}_h, \\ R'_{1,1} &= -\tau^2\mathbf{d}'(\mathbf{W}_h^2 - \mathbf{J}_{n+1})(\mathbf{I} + \tau^2\mathbf{A}'\mathbf{B}'(\mathbf{W}_h^2 - \mathbf{J}_{n+1}))^{-1}\mathbf{A}', \\ R'_{1,2} &= -\tau\mathbf{d}'(\mathbf{W}_h^2 - \mathbf{J}_{n+1})(\mathbf{I} + \tau^2\mathbf{A}'\mathbf{B}'(\mathbf{W}_h^2 - \mathbf{J}_{n+1}))^{-1}\mathbf{W}_h^{-1}, \\ W_h\xi_n &= R_{1,1}\mathbf{W}_h\mathbf{r}_n + R_{1,2}\mathbf{r}_{n+1/2} + W_h\rho_n, \\ \xi_{n+1/2} &= R'_{1,2}\mathbf{W}_h\mathbf{r}_{n+1} + R'_{1,1}\mathbf{r}'_{n+1/2} + \rho_{n+1/2}\end{aligned} \quad (33)$$

with  $\mathbf{I} = I_s \otimes I_m$ .

In order to prove the convergence, we introduce new variables following [6] and [15].

As in the proof of Lemma II.2.3 in [6] and 5.3 in [15], we put

$$\begin{aligned}\begin{pmatrix} W_h\nu_n \\ \nu_{n+1/2} \end{pmatrix} &= (R(\tau W_h) - I_{2m})^{-1}M(\tau W_h) \begin{pmatrix} W_h\psi_n \\ \psi_{n+1/2} \end{pmatrix} \\ &= \begin{pmatrix} [\mathbf{d}'(\mathbf{I} + \tau^2\mathbf{A}'\mathbf{B}'\mathbf{W}_h^2)^{-1}\mathbf{1}']^{-1}W_h^{-1}\tau^{-1}\psi_{n+1/2} \\ [\mathbf{d}(\mathbf{I} + \tau^2\mathbf{A}\mathbf{W}_h^2\mathbf{B})^{-1}\mathbf{1}']^{-1}W_h^{-1}\tau^{-1}W_h\psi_n \end{pmatrix},\end{aligned} \quad (34)$$

$$\begin{aligned}\begin{pmatrix} W_h\hat{\varepsilon}_n \\ \hat{\varepsilon}_{n+1/2} \end{pmatrix} &= \begin{pmatrix} W_h\varepsilon_n \\ \varepsilon_{n+1/2} \end{pmatrix} + \begin{pmatrix} W_h\nu_n \\ \nu_{n+1/2} \end{pmatrix}, \\ \begin{pmatrix} W_h\hat{\xi}_n \\ \hat{\xi}_{n+1/2} \end{pmatrix} &= \tau M(\tau W_h) \begin{pmatrix} W_h\bar{\xi}_n \\ \bar{\xi}_{n+1/2} \end{pmatrix} - \tau\bar{\mathbf{R}}_n \begin{pmatrix} W_h\nu_n \\ \nu_{n+1/2} \end{pmatrix} + \begin{pmatrix} W_h(\nu_{n+1} - \nu_n) \\ \nu_{n+3/2} - \nu_{n+1/2} \end{pmatrix}\end{aligned} \quad (35)$$

and rewrite (32) as

$$\begin{pmatrix} W_h\hat{\varepsilon}_{n+1} \\ \hat{\varepsilon}_{n+3/2} \end{pmatrix} = \mathbf{R}_n \begin{pmatrix} W_h\hat{\varepsilon}_n \\ \hat{\varepsilon}_{n+1/2} \end{pmatrix} + \begin{pmatrix} W_h\hat{\xi}_n \\ \hat{\xi}_{n+1/2} \end{pmatrix}. \quad (36)$$

Here

$$\begin{aligned}
M(\tau W_h) &= \begin{pmatrix} I_m & O \\ r'_{1,2}(\tau W_h) \mathbf{1}' & I_m \end{pmatrix}, \\
W_h \psi_n &= r_{1,1}(\tau W_h) \mathbf{W}_h \mathbf{r}_n + r_{1,2}(\tau W_h) \mathbf{r}_{n+1/2} + W_h \rho_n, \\
\psi_{n+1/2} &= r'_{1,2}(\tau W_h) \mathbf{W}_h \mathbf{r}_{n+1} + r'_{1,1}(\tau W_h) \mathbf{r}'_{n+1/2} + \rho_{n+1/2}, \\
W_h \bar{\xi}_n &= \bar{R}_{1,1} \mathbf{W}_h \mathbf{r}_n + \bar{R}_{1,2} \mathbf{r}_{n+1/2}, \\
\bar{\xi}_{n+1/2} &= \bar{R}'_{1,2} \mathbf{1}' W_h \bar{\xi}_n + \bar{R}'_{1,2} \mathbf{W}_h \mathbf{r}_{n+1} + \bar{R}'_{1,1} \mathbf{r}'_{n+1/2}.
\end{aligned} \tag{37}$$

$\bar{\mathbf{R}}_n$  is defined as  $\tau \bar{\mathbf{R}}_n = \mathbf{R}_n - R(\tau W_h)$ , given by

$$\bar{\mathbf{R}}_n = \begin{pmatrix} \bar{R}_{1,1} \mathbf{1}' & \bar{R}_{1,2} \mathbf{1}' \\ R'_{1,2} \mathbf{1}' \bar{R}_{1,1} \mathbf{1}' + \bar{R}'_{1,2} \mathbf{1}' & R'_{1,2} \mathbf{1}' \bar{R}_{1,2} \mathbf{1}' + \bar{R}'_{1,2} \mathbf{1}' r_{1,2}(\tau W_h) \mathbf{1}' + \bar{R}'_{1,1} \mathbf{1}' \end{pmatrix}.$$

Since  $\mathbf{A} \mathbf{W}_h^2 \mathbf{B} = \mathbf{W}_h^2 \mathbf{A} \mathbf{B}$ ,  $\mathbf{A}' \mathbf{B}' \mathbf{W}_h^2 = \mathbf{W}_h^2 \mathbf{A}' \mathbf{B}'$ ,  $\bar{R}_{1,i}$ ,  $\bar{R}'_{1,i}$ ,  $i = 1, 2$  are written as

$$\begin{aligned}
\bar{R}_{1,1} &= -\tau \mathbf{d} \sum_{i=0}^{s-1} (-1)^i \{ (\tau^2 \mathbf{W}_h^2 \mathbf{A} \mathbf{B} - \tau^2 \mathbf{A} \mathbf{J}_n \mathbf{B})^i - (\tau^2 \mathbf{W}_h^2 \mathbf{A} \mathbf{B})^i \} \mathbf{A} \mathbf{W}_h^2 \\
&\quad + \tau \mathbf{d} \sum_{i=0}^{s-1} (\tau^2 \mathbf{A} (\mathbf{J}_n - \mathbf{W}_h^2) \mathbf{B})^i \mathbf{A} \mathbf{J}_n, \\
\bar{R}_{1,2} &= \mathbf{d} \sum_{i=0}^{s-1} (-1)^i \{ (\tau^2 \mathbf{W}_h^2 \mathbf{A} \mathbf{B} - \tau^2 \mathbf{A} \mathbf{J}_n \mathbf{B})^i - (\tau^2 \mathbf{W}_h^2 \mathbf{A} \mathbf{B})^i \} \mathbf{W}_h, \\
\bar{R}'_{1,1} &= -\tau \mathbf{d}' \mathbf{W}_h^2 \sum_{i=0}^{s-1} (-1)^i \{ (\tau^2 \mathbf{W}_h^2 \mathbf{A}' \mathbf{B}' - \tau^2 \mathbf{A}' \mathbf{B}' \mathbf{J}_{n+1})^i - (\tau^2 \mathbf{W}_h^2 \mathbf{A}' \mathbf{B}')^i \} \mathbf{A}' \\
&\quad + \tau \mathbf{d}' \mathbf{J}_{n+1} \sum_{i=0}^{s-1} (\tau^2 \mathbf{A}' \mathbf{B}' (\mathbf{J}_{n+1} - \mathbf{W}_h^2))^i \mathbf{A}', \\
\bar{R}'_{1,2} &= -\mathbf{d}' \mathbf{W}_h \sum_{i=0}^{s-1} (-1)^i \{ (\tau^2 \mathbf{W}_h^2 \mathbf{A}' \mathbf{B}' - \tau^2 \mathbf{A}' \mathbf{B}' \mathbf{J}_{n+1})^i - (\tau^2 \mathbf{W}_h^2 \mathbf{A}' \mathbf{B}')^i \} \\
&\quad + \mathbf{d}' \mathbf{J}_{n+1} \sum_{i=0}^{s-1} (\tau^2 \mathbf{A}' \mathbf{B}' (\mathbf{J}_{n+1} - \mathbf{W}_h^2))^i \mathbf{W}_h^{-1}.
\end{aligned}$$

By (31) and (H6), we can estimate  $\bar{R}_{1,i}$ ,  $\bar{R}'_{1,i}$ ,  $i = 1, 2$  as

$$\bar{R}_{1,i} = O(\tau), \quad \bar{R}'_{1,1} = O(\tau), \quad \bar{R}'_{1,2} = O(1). \tag{39}$$

Substituting (30) into (33) and (38), we get

$$\left\| (\bar{\xi}_n, \bar{\xi}_{n+1/2})^T \right\|_{W_h} \leq C_1 \left( \tau^2 + \max_{i=0,1} \|\alpha_h(t_{n+i})\| \right) \tag{40}$$

with a positive constant  $C'_1$ .

For  $\theta \in S'$ , there exist some positive constants  $\gamma_4, \gamma'_4$  such that,  $r_{1,2}(\theta)\mathbf{1}/\theta = d(I_s + \theta^2 AB)^{-1}\mathbf{1} > \gamma_4$  and  $-r'_{1,2}(\theta)\mathbf{1}/\theta = d'(I_s + \theta^2 A'B')^{-1}\mathbf{1} > \gamma'_4$ . By (H6), any eigenvalue of  $[d(\mathbf{I} + \tau^2 \mathbf{W}_h^2 \mathbf{A} \mathbf{B})^{-1} \mathbf{1}']^{-1}$  and  $[d'(\mathbf{I} + \tau^2 \mathbf{W}_h^2 \mathbf{A}' \mathbf{B}')^{-1} \mathbf{1}']^{-1}$  are less than  $\gamma_4$  and  $\gamma'_4$ , respectively. Substituting (30) into (37),  $W_h^{-1} \tau^{-1} W_h \psi_n$  and  $W_h^{-1} \tau^{-1} \psi_{n+1/2}$  are represented as

$$\begin{aligned} W_h^{-1} \tau^{-1} W_h \psi_n &= r_{1,2}(\tau W_h) \mathbf{A} \boldsymbol{\alpha}_h(t_n) + O(\tau^2), \\ W_h^{-1} \tau^{-1} \psi_{n+1/2} &= (r'_{1,1}(\tau W_h) \mathbf{B}' + \mathbf{d}') \boldsymbol{\alpha}_h(t_{n+1}) + O(\tau^2). \end{aligned} \quad (41)$$

Substituting (41) into (34), there is a positive constant  $C''_1$  such that

$$\left\| (\nu_n, \nu_{n+1/2})^T \right\|_{W_h} \leq C''_1 \left( \tau^2 + \max_{i=0,1} \|\alpha_h(t_{n+i})\| \right). \quad (42)$$

Since  $\mathbf{u}_h^{(3)}(t_{n+1}) - \mathbf{u}_h^{(3)}(t_n) = O(\tau)$  and  $\mathbf{v}_h^{(3)}(t_{n+3/2}) - \mathbf{v}_h^{(3)}(t_{n+1/2}) = O(\tau)$ , we get

$$\begin{aligned} W^{-1} \tau^{-1} W_h (\psi_{n+1} - \psi_n) &= \tau r_{1,2}(\tau W_h) \mathbf{A} \{\boldsymbol{\alpha}_h(t_{n+1}) - \boldsymbol{\alpha}_h(t_n)\} + O(\tau^3), \\ W^{-1} \tau^{-1} (\psi_{n+3/2} - \psi_{n+1/2}) &= \tau (r'_{1,1}(\tau W_h) \mathbf{B}' + \mathbf{d}') \{\boldsymbol{\alpha}_h(t_{n+2}) - \boldsymbol{\alpha}_h(t_{n+1})\} + O(\tau^3). \end{aligned}$$

Thus, by using (35), (40) and (42), there is a positive constant  $C_2$  such that

$$\left\| (\hat{\xi}_n, \hat{\xi}_{n+1/2})^T \right\|_{W_h} \leq C_2 \left( \tau^3 + \tau \max_{i=0,1} \|\alpha_h(t_{n+i})\| \right). \quad (43)$$

Moreover, let  $\omega_j$  be the eigenvalues of  $W_h$ . Then, by taking the orthogonal matrix  $P$  to be  $P^{-1}(\tau W_h)P = \text{diag}(\tau \omega_j)$ , we have

$$R(\tau W_h) = \mathbf{P} R(\text{diag}(\tau \omega_j)) \mathbf{P}^{-1}, \text{ where } \mathbf{P} = I_2 \otimes P.$$

Here  $R(\text{diag}(\tau \omega_j))$  is the same formula as (10), replacing  $\theta$  by  $\text{diag}(\tau \omega_j)$ . Let  $\lambda_{\pm}(\tau \omega_j) = \lambda_{\pm j}$  be the eigenvalues of  $R(\text{diag}(\tau \omega_j))$ .  $\lambda_{\pm j}$  are the solutions of (12), replacing  $\theta$  by  $\tau \omega_j$ . By (H6), we have  $0 \leq \tau \omega_j < \gamma_0$  and  $|\lambda_{\pm j}| \leq 1$ ,  $j = 1, \dots, m$ . Then, by using Theorem 3.1, we obtain

$$\|R(\tau W_h)^n\| = \|R(\text{diag}(\tau \omega_j))^n\| \leq K \quad (44)$$

with  $K$  a constant independent of  $n \in \mathbb{N}$ ,  $\tau$  and  $h$ ,  $\|\cdot\|$  denotes the operator norm for  $2m \times 2m$  matrices.

By (39), we obtain

$$\|\bar{\mathbf{R}}_n\| \leq K_1, \quad (45)$$



where  $K_1$  is a constant independent of  $n$ ,  $\tau$  and  $h$ .  
From (44) and (45), we obtain

$$\left\| \prod_{i=1}^n \mathbf{R}_i \right\| \leq \|R(\tau W_h)^n\| (1 + \tau K_1)^n \leq K e^{n\tau K_1} \leq K_2. \quad (46)$$

Hence, from (36), (43) and (46), we obtain

$$\left\| (\hat{\varepsilon}_n, \hat{\varepsilon}_{n+1/2})^T \right\|_{W_h} \leq K_2 \left\| (\hat{\varepsilon}_0, \hat{\varepsilon}_{1/2})^T \right\|_{W_h} + K_2 n C_2 \left( \tau^3 + \tau \max_{0 \leq t \leq T} \|\alpha_h(t)\| \right),$$

which implies that

$$\left\| (\hat{\varepsilon}_n, \hat{\varepsilon}_{n+1/2})^T \right\|_{W_h} \leq K_2 \left\| (\nu_0, \varepsilon_{1/2} + \nu_{1/2})^T \right\|_{W_h} + K_2 T C_2 \left( \tau^2 + \max_{0 \leq t \leq T} \|\alpha_h(t)\| \right)$$

for  $1 \leq n \leq N$ . Using  $\left\| (\nu_0, \varepsilon_{1/2} + \nu_{1/2})^T \right\|_{W_h} = C'_2 \tau^2$  for a constant  $C'_2 > 0$ ,

$$\left\| (\varepsilon_n, \varepsilon_{n+1/2})^T \right\|_{W_h} \leq \left\| (\hat{\varepsilon}_n, \hat{\varepsilon}_{n+1/2})^T \right\|_{W_h} + \left\| (\nu_n, \nu_{n+1/2})^T \right\|_{W_h}$$

and rewriting the constants, we finally obtain (28).  $\square$

## 5 Numerical experiments

We examine the convergence of the leapfrog scheme (13) and RKS4 (15), by using the following model problem

$$\begin{aligned} \frac{\partial u}{\partial t} &= v, \quad \frac{\partial v}{\partial t} = \frac{\partial^2 u}{\partial x^2} + g(t, x, u), \quad 0 \leq t \leq T, \quad x \in \Omega, \\ u(t, 0) &= \beta_0(t), \quad u(t, 1) = \beta_1(t), \quad 0 \leq t \leq T, \\ u(0, x) &= u_0(x), \quad \frac{\partial u}{\partial t}(0, x) = v_0(x), \quad x \in \Omega. \end{aligned} \quad (47)$$

Here  $T = 1$ ,  $\Omega = [0, 1]$ ,  $g(t, x, u) = -\sin u$  and  $\beta_0(t)$ ,  $\beta_1(t)$ ,  $u_0(x)$  and  $v_0(x)$  are given by using the following exact solution ([13])

$$u(t, x) = 4 \tan^{-1} \left\{ \gamma \sinh \left( \frac{x}{\sqrt{1 - \gamma^2}} \right) / \cosh \left( \frac{\gamma t}{\sqrt{1 - \gamma^2}} \right) \right\}$$

with  $\gamma = 0.5$ . Let  $N$  be a positive integer,  $h = 1/N$ , and  $\Omega_h$  be a uniform grid with nodes  $x_j = jh$ ,  $j = 0, 1, \dots, N$ . We discretize  $\frac{\partial v}{\partial t} = \frac{\partial^2 u}{\partial x^2} + g(t, x, u)$  in space with

the fourth-order implicit scheme

$$\begin{aligned} \frac{1}{12} \left\{ \frac{dv^{j-1}(t)}{dt} + 10 \frac{dv^j(t)}{dt} + \frac{dv^{j+1}(t)}{dt} \right\} &= \frac{1}{h^2} \{u^{j-1}(t) - 2u^j(t) + u^{j+1}(t)\} \\ &- \frac{1}{12} \{ \sin u^{j-1}(t) + 10 \sin u^j(t) + \sin u^{j+1}(t) \} \end{aligned}$$

with  $u^j(t) \approx u(t, x_j)$ ,  $v^j(t) \approx v(t, x_j)$  (see, [16]). Putting

$$u_h(t) = (u^0(t), \dots, u^N(t))^T, \quad v_h(t) = (v^0(t), \dots, v^N(t))^T,$$

we obtain the MOL approximation

$$\frac{du_h(t)}{dt} = v_h(t), \quad \hat{H} \frac{dv_h(t)}{dt} = \hat{L}_h u_h(t) + \hat{\varphi}_h(t) + \hat{H} g_h(t, u_h(t)), \quad (48)$$

where

$$\hat{L}_h = \frac{1}{h^2} \begin{pmatrix} -2 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \cdots & 0 \\ 0 & 1 & -2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 & -2 \end{pmatrix}, \quad \hat{H} = \frac{1}{12} \begin{pmatrix} 10 & 1 & 0 & \cdots & 0 \\ 1 & 10 & 1 & \cdots & 0 \\ 0 & 1 & 10 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 & 10 \end{pmatrix},$$

and  $\hat{\varphi}_h(t) = (\beta_0(t), 0, \dots, 0, \beta_1(t))^T$ . The eigenvalues of  $\hat{L}_h$  and  $\hat{H}$  are

$$\frac{2}{h^2} \left( \cos \frac{(j+1)\pi}{N+2} - 1 \right), \quad \frac{1}{6} \left( 5 + \cos \frac{(j+1)\pi}{N+2} \right), \quad j = 0, 1, \dots, N, \quad (49)$$

respectively.

Multiplying  $\hat{H}^{-1}$  to (48), we get (2) with  $D = 1$ ,  $L_h = \hat{H}^{-1} \hat{L}_h$ ,  $\varphi_h(t) = \hat{H}^{-1} \hat{\varphi}_h(t)$ . By (49) the eigenvalues of  $L_h$  are

$$\frac{12}{h^2} \left( 1 - \frac{6}{5 + \cos((j+1)\pi/(N+2))} \right), \quad j = 0, 1, \dots, N.$$

Since

$$\tau \rho(W_h) = \frac{2\sqrt{3}\tau}{h} \left( \frac{6}{5 + \cos((N+1)\pi/(N+2))} - 1 \right)^{\frac{1}{2}} < \frac{\sqrt{6}\tau}{h},$$

if we take the step size  $\tau < \sqrt{2}h/\sqrt{3}$ , (H6) holds for the leapfrog scheme. If we take the step size  $\tau < 2h$ , (H6) holds for RKS4. We take the spatial step size  $h$  and temporal step size  $\tau$  such that  $h = 2\tau = 1/N$  so that both conditions are

satisfied. We apply the leapfrog scheme and RKS4 to the MOL approximation (48), and integrate from  $t = 0$  to  $t = T$ . We measure the errors of the schemes by using the discrete  $L_2$ -norm

$$\varepsilon_{u,L2} = \max_{0 < n \leq 2NT} \|\varepsilon_n\|, \quad \varepsilon_{v,L2} = \max_{0 < n \leq 2NT} \|\varepsilon_{n+1/2}\|,$$

the discrete energy norm

$$\varepsilon_e = \max_{0 < n \leq 2NT} \|(\varepsilon_n, \varepsilon_{n+1/2})\|_{W_h}$$

and maximum norm

$$\varepsilon_{u,\max} = \max_{0 < n \leq 2NT} \{\|\varepsilon_n\|_\infty\}, \quad \varepsilon_{v,\max} = \max_{0 < n \leq 2NT} \{\|\varepsilon_{n+1/2}\|_\infty\}$$

with  $\|\cdot\|_\infty$  the maximum norm on  $\mathbb{R}^m$ .

Table 1: Numerical results for (47) using the leapfrog scheme

$N$	10	20	40	80	160	320	640
$-\log_2 \varepsilon_{u,L2}$	16.04	18.15	20.17	22.18	24.18	26.18	28.18
Increment		2.11	2.02	2.01	2.00	2.00	2.00
$-\log_2 \varepsilon_{v,L2}$	14.10	16.13	18.14	20.14	22.15	24.15	26.15
Increment		2.03	2.01	2.00	2.01	2.00	2.00
$-\log_2 \varepsilon_{u,\max}$	15.55	17.66	19.68	21.69	23.69	25.69	27.69
Increment		2.11	2.02	2.01	2.00	2.00	2.00
$-\log_2 \varepsilon_{v,\max}$	13.70	15.75	17.76	19.77	21.77	23.77	25.77
Increment		2.05	2.01	2.01	2.00	2.00	2.00
$-\log_2 \varepsilon_e$	13.31	15.40	17.42	19.42	21.43	23.43	25.43
Increment		2.09	2.02	2.00	2.01	2.00	2.00

Table 2: Numerical results for (47) using RKS4

$N$	10	20	40	80	160	320	640
$-\log_2 \varepsilon_{u,L2}$	19.17	23.16	27.15	31.15	35.15	39.15	43.14
Increment		3.99	3.99	4.00	4.00	4.00	3.99
$-\log_2 \varepsilon_{v,L2}$	18.28	22.27	26.23	29.67	32.24	34.74	37.14
Increment		3.99	3.96	3.44	2.57	2.50	2.40
$-\log_2 \varepsilon_{u,\max}$	18.73	22.71	26.70	30.70	34.70	38.70	42.62
Increment		3.98	3.99	4.00	4.00	4.00	3.92
$-\log_2 \varepsilon_{v,\max}$	17.51	21.51	24.62	26.60	28.59	30.59	32.57
Increment		4.00	3.11	1.98	1.99	2.00	1.98
$-\log_2 \varepsilon_e$	16.98	20.97	24.90	28.60	31.75	34.55	36.73
Increment		3.99	3.93	3.70	3.15	2.80	2.18

Table 1 and Table 2 show that the observed order of the leapfrog scheme and RKS4 are more than or equal to 2. We observe that the order for  $u$  of RKS4 is higher than expected results from Theorem 4.1.

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